Acetone
67-64-1 | DTXSID8021482

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.59 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.83e-01

Confidence level: 6.81e-01

Nearest Neighbors from the Training Set

Image not found
Acetone
Measured: 17.2
Predicted: 6.59

Image not found
Acrolein
Measured: 3.78
Predicted: 5.11

Image not found
Methyl ethyl ketone
Measured: 3.09
Predicted: 2.13

Image not found
Methacrylaldehyde
Measured: 8.08e-01
Predicted: 2.22

Image not found
Propanal
Measured: 5.27
Predicted: 3.91